Comparison between two methods of solution of coupled equations for low-energy scattering

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Cross sections from low-energy neutron-nucleus scattering have been evaluated using a coupled channel theory of scattering. Both a coordinate-space and a momentum-space formalism of that coupled-channel theory are considered. A simple rotational model of the channel interaction potentials is used to find results using two relevant codes, ECIS97 and MCAS, so that they may be compared. The very same model is then used in the MCAS approach to quantify the changes that occur when allowance is made for effects of the Pauli principle.

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I. INTRODUCTION

In analyses of low-energy scattering data and in forming evaluated nuclear data files, much use has been made of programs designed to solve equations of coupled channels scattering theory. Programs such as CHUCK [1] and ECIS [2, 3] seek such solutions using a coordinate space representation of the scattering. Versions of ECIS in fact are embedded within, or used with, such large scale analysis programs as GNASH [4], EMPIRE-II [5] and TALYS [6], providing basic input for the diverse evaluations they make. These codes, the ECIS codes in particular, use collective model prescriptions for the coupling interactions with deformation taken to second order for some cases.

It has long been known [7, 8] that using these collective model prescriptions violate the Pauli principle, and it has also been argued that such violations could not be avoided. However, it was shown recently [9] how the Pauli principle could be satisfied with a method of solution of the coupled-channels problem built in momentum space using separable expansions of the coupling interactions. That multi-channel algebraic scattering (MCAS) theory [10] when formed using Sturmians that are orthogonal to any Pauli blocked state as the expansion basis, gave excellent results for both the scattering cross sections and sub-threshold spectra for the examples considered: protons and neutrons on ^{12}C. To create the appropriate set of Sturmians, an orthogonalizing pseudopotential (OPP) method was used [10]. Violation of the Pauli principle was shown to have serious effect on results. That raises concern about the application of interactions and wave functions generated by neglecting the Pauli principle when interactions have been adjusted to give fits to low-energy scattering data.

Herein, we report on a comparative study of the results of using a coordinate space program (ECIS97) and MCAS (with and without taking into account the Pauli principle) to see if a) the calculations are the same when one seeks to perform the exact same evaluation with each, b) for a typical low energy problem, how the Pauli principle influences the results, and c) what underlying structure of the compound system is inferred.

To compare the results of the two codes, we have used a simple (test) model for the neutron-^{12}C system. We allow three target states to define the coupled channels in both the coordinate space (ECIS97) and the momentum space (MCAS) evaluations. They are the ground (0^+), first excited state (2^+; 4.43 MeV), and the second excited state (0_2^+; 7.67 MeV). We also assume that the coupling is effected by a simple rotational model scheme having only a quadrupole deformation with $\beta_2 = -0.52$ upon a purely real spherical Woods-Saxon potential [3] given in MeV. All length parameters are expressed in fm, and the

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deformed field form is

$$V(r) = -49.92\, f(r) + \left(\frac{\hbar}{m_\pi c}\right)^2 6\,\sigma\cdot\nabla f(r)\times\frac{1}{i}\nabla \quad (1)$$

$$f(r) = \left[1+\exp\left(\frac{r-2.885}{0.63}\right)\right]^{-1} . \quad (2)$$

In the MCAS evaluation the spin-orbit term is reduced to the $\mathbf{l}\cdot\mathbf{s}$ form. This potential is fixed for all calculations that we have made and whose results are reported herein.

For the comparative study of $n+^{12}$C in a rotational model, MCAS carries the deformation up to second order. ECIS [2, 3] allows deformation to second order with various vibration model specifications of the channel interactions, but with the rotation model, the expansion of the nuclear deformation is only taken to first order.

II. GENERAL REMARKS ABOUT ECIS AND MCAS

Details of what these two codes calculate are presented in the literature and so only brief comment is given here. For ECIS we refer the reader to the documentation [2, 3] for a more detailed description. With MCAS there are three publications to consider. The first [10] gives a detailed description of the method and the model interactions chosen for the application made. The second [9] highlights how that process corrects a collective model prescription of the scattering to allow for the Pauli principle, and therein it is shown just how crucial that is if a physically significant interaction is to be defined. Finally, in Ref. [11] the physics that can be extracted by using the MCAS scheme is highlighted, but only when the Pauli principle effects are treated.

ECIS97 has been constructed to use a wide range of (collective) model structures to describe the nuclear interaction matrices of potentials, $V_{c'c}(r)$. MCAS on the other hand is still in its infancy and to date the only working program is one that inputs a rotational (collective) model matrix of potentials. Development to incorporate a vibration model for the target spectrum as well as to use shell model wave functions to define the matrices of coupling potentials is proceeding. However, to make a comparison between two codes we consider only the case of a simple rotation model scheme.

We specify the complete channel index by $c:(\ell(\frac{1}{2})j, I; J^\pi)$, which couples the incident partial wave angular momenta $\{\ell(\frac{1}{2})j\}$ to the target spin I to get the total system spin-parity J^π. The last is conserved in the scattering process. ECIS97 solves the coupled-channels problem in coordinate space so that the defining equations have the form (Eq. (17) in Ref. [2]),

$$\frac{\hbar^2}{2\mu}\left[\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}+k^2\right] f_c(r) = \sum_{c'} V_{c,c'}(r)\, f_{c'}(r) \ , \quad (3)$$

where the notation is as usual. As noted [2], the wave functions $f_c(r)$ have asymptotic forms for large r (Eq. (8) in Ref. [2])

$$f_{l,j}(r) = F_l(\eta, kr) + C_{l,j}\left[G_l(\eta,kr) + iF_l(\eta,kr)\right] \ , \quad (4)$$

where, with η being the Sommerfeld parameter, F_l, G_l are the regular and irregular (at the origin) Coulomb functions. The solutions in the case of closed channels are the appropriate decaying forms.

With the rotational model for the matrices of potentials, in ECIS97 a first order multipole expansion is considered, namely

$$R = R_0\left[1+\sum_\lambda \beta_\lambda Y^\star_{\lambda,0}(\Omega_A)\right] , \quad (5)$$

so that the operator form of the projectile-nucleus interactions becomes

$$V(r,\Omega_A) = V_0(r) + \sum_\lambda V_\lambda(r)\mathbf{Y}^\star_\lambda(\Omega_A)\cdot\mathbf{Y}_\lambda(\Omega_r) \ . \quad (6)$$

When only the quadrupole moment defines the test model, an ECIS97 run should then coincide with an MCAS calculation in which deformation is limited to first order.

The details of the MCAS approach are published in Ref. [10], and so we do not repeat them here. It suffices to note that deformation of the interaction from the rotation model is taken to second order and the program allows flexibility in the forms; permitting parity, orbital angular momentum, and target spin dependences. For the test model calculations, the results of which are reported herein, such flexibility has not been exploited.

III. RESULTS AND DISCUSSION

The program ECIS97 was run for the test model at a series of (laboratory) energies E_{lab} from 0.1 MeV to 4.0 MeV. The results are displayed in Fig. 1 by the filled circles connected by a (spline) curve and reveal three resonances near 0.7, 2.1, and 3.3 MeV. The solid curve in that figure is the cross section found from ECIS97 calculations made using the same spherical potential but considering only the elastic channel. That is the basic optical model result in which there is a shape, or single particle, resonance centered about $E_{\rm lab} = 2$ MeV. Clearly the inclusion of channel coupling changes these cross sections significantly. So the results we compare next are ones of a significant coupled channel problem and not ones that might be obtained simply by adjustments of the parametric form of the ground state (optical) potential.

ECIS calculations usually are made with the full Thomas form of the spin-orbit interaction. However in the write-up of that code [2] it is shown how one can limit calculations so that the $\mathbf{l}\cdot\mathbf{s}$ form is used. That form is

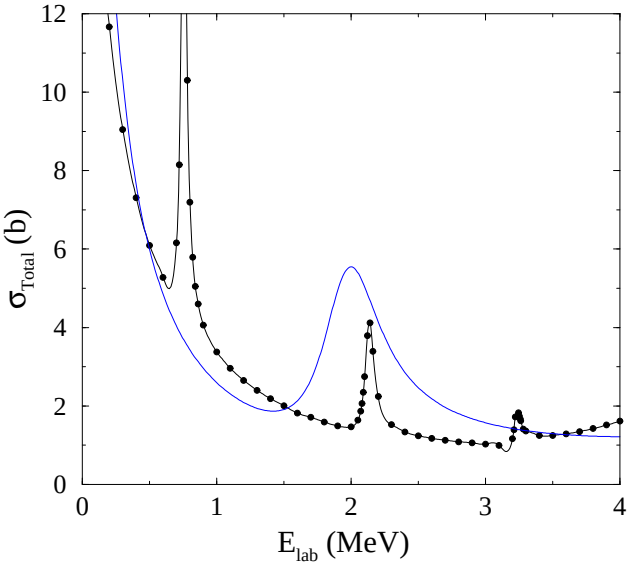

FIG. 1: (Color online) The results from using ECIS97 to evaluate the test model cross sections for the $n+^{12}$C system. The filled circles connected by a line is the cross section found from the ECIS coupled channels calculations while the solid curve is the result when coupling is set to zero (the ground state potential scattering calculation).

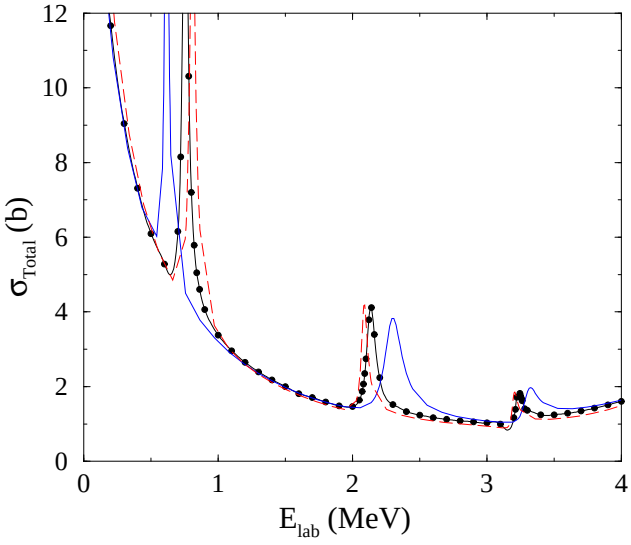

FIG. 2: (Color online) The $n+^{12}$C cross section results from using MCAS theory to first order in deformation (dashed curve) and for deformation taken to second order (solid curve), compared with those found by using the ECIS97 program (filled circles connected by a line).

what we have incorporated (so far) in MCAS. We have made ECIS calculations both with the full Thomas and with the $\mathbf{l}\cdot\mathbf{s}$ forms. The two calculated cross sections are in very good agreement for most of the energy range and only the strong low-energy $\frac{5}{2}^+$ resonance is slightly shifted in its centroid by the reduction to the simplest spin-orbit form. These results corroborate findings in previous studies [12] that only at higher energies, and for observables directly linked to inelastic-channel interactions, does use of the full Thomas term rather than the $\mathbf{l}\cdot\mathbf{s}$ form have some effect. Even then, those effects are very small and essentially with the forward angle spin dependent observables, such as the analyzing powers.

First MCAS calculations have been made using the same test model, and the fixed interaction given in Eq. (1) but with the $(\mathbf{l}\cdot\mathbf{s})$ form for the spin-orbit components and without accounting for the Pauli principle. In Fig. 2, these results are compared with those found using the ECIS97 code. The ECIS results again are displayed by the filled circles connected by a solid line and there are two MCAS results. The first, displayed by the solid curve, involved deformation taken through second order [10]. It agrees with the background found from the ECIS calculation and also has the same three resonances though their energy centroids are shifted. The second MCAS result, depicted by the dashed curve, was obtained by limiting deformation to first order. This result is in better agreement with the ECIS cross section, both background and resonances (centroids and widths). Slight differences must be allowed since the two codes involve quite different numerics and associated accuracies. We consider the whole set of results to be close enough to claim that the two codes are equivalent in what they evaluate.

Two conclusions may be drawn from the results found so far. First, when the test model is used in exactly the same way in finding solutions of the coupled-channel problem using the coordinate space approach [2] and the momentum space approach with MCAS [10], the scattering cross sections agree very well. The smooth background as well as the specific resonances that can be generated with ECIS are found with the MCAS run. The second conclusion evident from comparison of the two MCAS results is that, with deformation of $\beta_2 = -0.52$ which is realistic for the actual system, a first order approach is insufficient.

We have shown that the two programs evaluate equivalent cross sections but those evaluations are equivalently in error as the effects of the Pauli principle [9] have been ignored. We now consider just how important it is to include the Pauli principle and how the associated blocking mechanism works with this test model. As noted earlier, in the MCAS approach, an OPP method can be used to ensure that there is no violation of the Pauli principle. The OPP method ensures that the Sturmians used an expansion set in the MCAS approach are orthogonal to all states in which the incoming nucleon would be trapped into an orbit fully occupied by nucleons in the target. Using such a conditioned Sturmian function set to solve the MCAS theory of coupled equations gives the cross section displayed by the solid curve in Fig. 3. That is compared with the MCAS result shown previously and found without using the OPP and taking deformation

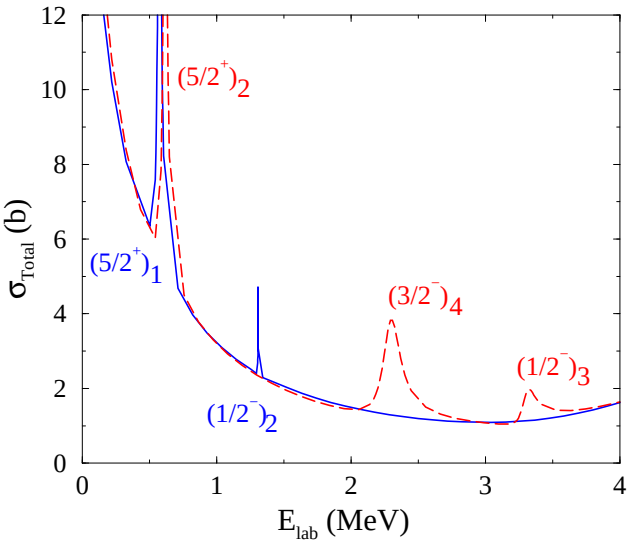

FIG. 3: (Color online) The $n + {}^{12}$C cross section results from using MCAS theory with (solid curve) and without (dashed curve) using the OPP method to prevent violation of the Pauli principle.

also to second order. That latter result is portrayed by the dashed curve in Fig. 3. The changes seen are dramatic.

To discuss them, first it is important to note that the MCAS theory [10] embodies a resonance finding scheme with which all subthreshold and resonance states, no matter how narrow any of the latter may be, that lie within any energy range selected for study will be found and their spin-parities, energy centroids, and widths determined. Furthermore the order number of each can be obtained. The order number (r) identifies that there are $r-1$ bound states/resonances of that given J^π lying below in the spectrum of the compound system. In Fig. 3 then, each resonance is identified by its value of $(J^\pi)_r$. While the background cross section calculated with and without Pauli blocking is essentially unchanged, the resonance properties are drastically altered. Both calculations give a $\frac{5}{2}^+$ resonance near 0.6 MeV but the number order differs. Then, the $\frac{3}{2}^-$ resonance disappears while the $\frac{1}{2}^-$ resonance relocates to lower energy, changes its order number to 2, and has a much narrower width when the effects of the Pauli principle are considered. The prime effect of including the Pauli principle is to remove numerous spurious states from the spectrum. However, it also changes the underlying structure of what states remain [11]. In that reference, the tracking of states and resonances as deformation is decreased to zero revealed the basic origin of each state and resonance. With the test model, set so that a direct comparison between two methods of solving coupled channels problems can be made, we show in Table I, the full spectra that have been obtained using MCAS with and without the OPP and in the zero deformation limit. This table is similar to that given previously [11] and which was found with a matrix of interaction potentials that gave an excellent fit to data. However, it is important to present these values, not only as they are specifically those from the test model we have used, but also as some of the values bear upon conclusions to be drawn from the results shown in Fig. 3.

TABLE I: The spectra found with MCAS when $\beta_2 \longrightarrow 0$. In the first column, the numerical labels for the spurious states are presented in the brackets, {n}. The arrows in the second column indicate the Pauli-allowed states obtained when the OPP is applied. The subscript r is the order number of each state and resonance.

label	$(J)^\pi_r$	Energy	$^{12}\mathrm{C} + (n\ell_j)$
{1}	$\left(\frac{1}{2}\right)^+_1$	-23.50	$0^+_1 + 0s_{\frac{1}{2}}$
{2}	$\left(\frac{3}{2}\right)^+_1, \left(\frac{5}{2}\right)^+_1$	-19.07	$2^+_1 + 0s_{\frac{1}{2}}$
{3}	$\left(\frac{1}{2}\right)^+_2$	-15.85	$0^+_2 + 0s_{\frac{1}{2}}$
{4}	$\left(\frac{3}{2}\right)^-_1$	-9.73	$0^+_1 + 0p_{\frac{3}{2}}$
5	$\left(\frac{1}{2}\right)^-_1 \rightarrow \left(\frac{1}{2}\right)^-_1$	-5.92	$0^+_1 + 0p_{\frac{1}{2}}$
{6}	$\left(\frac{1}{2}\right)^-_2, \left(\frac{3}{2}\right)^-_2, \left(\frac{5}{2}\right)^-_1, \left(\frac{7}{2}\right)^-_1$	-5.29	$2^+_1 + 0p_{\frac{3}{2}}$
{7}	$\left(\frac{3}{2}\right)^-_3$	-2.07	$0^+_2 + 0p_{\frac{3}{2}}$
8	$\left(\frac{3}{2}\right)^-_4, \left(\frac{5}{2}\right)^-_2 \rightarrow \left(\frac{3}{2}\right)^-_1, \left(\frac{5}{2}\right)^-_1$	-1.48	$2^+_1 + 0p_{\frac{1}{2}}$
9	$\left(\frac{1}{2}\right)^-_3 \rightarrow \left(\frac{1}{2}\right)^-_2$	1.74	$0^+_2 + 0p_{\frac{1}{2}}$
10	$\left(\frac{5}{2}\right)^+_2 \rightarrow \left(\frac{5}{2}\right)^+_1$	2.08	$0^+_1 + 0d_{\frac{5}{2}}$

For simplicity of discussion each state or group of states at a given value are identified by a label number in the first column. The states associated with labels set in curly brackets arise from Pauli violation and are numerically removed by the OPP method. In the second column the arrow indicates the Pauli-allowed states, all but the lowest of which are reduced in order number due to Pauli blocking. The energy gaps between, and spin-parities of, these states lead to the base prescription given in the column on the far right of Table I. The energy gaps in the zero deformation limit relate directly to the target spectrum values and the single nucleon state binding energies. Of relevance in this discussion is that the $\left(\frac{1}{2}^-\right)_2$ state in group labelled {6} is spurious. The allowed state $\left(\frac{1}{2}^-\right)_3$ of the set (the entry in group 9 in Table I) then becomes the $\left(\frac{1}{2}^-\right)_2$ state after application of the OPP method. Hence there is the reduction in order number of the calculated resonance state of that spin-parity shown in Fig. 3. Moreover, and associated with the removal of a basic spurious state of that spin-parity, with finite deformation forming admixtures to yield the end result, there will be no spurious component then in the resultant narrow resonance centered near 1.3 MeV. The change in character of that resonance due to the Pauli principle is evident. Likewise the lowest three $\frac{3}{2}^-$ states also are Pauli forbidden so the remaining allowed state is one of

the subthreshold compound nuclear states and there is no resonance of that spin-parity in the resultant cross section in contradiction to the result found without taking the Pauli principle into account. Finally there is one spurious $\frac{5}{2}^+$ state in the spectrum that has been removed and as the remaining state of that spin-parity is basically built as the $0d_{\frac{5}{2}}$ neutron coupled to the ground state of ^{12}C, there is no great change in centroid energy when the Pauli principle is considered. So, there are many spurious states when the Pauli principle is violated. Worse, there are spurious states having the same spin-parities as those to be found when the Pauli principle is preserved in the calculations. With deformation coupling, these basis states mix to determine that to be deemed the physical result.

If either code (used without Pauli correction) found that the simple interaction actually gave fits to cross-section data, then that interaction and, more importantly, the relative wave functions derived from it, would be wrong. One would need to invoke the OPP approach (or an equivalent) and then make a further parameter search to find an interaction that leads to a fit to the data. But it is important to note that the background cross section itself does not provide selectivity as it is dominated by s-wave scattering.

IV. CONCLUSIONS

In this paper we have compared the results when two different coupled-channel approaches (MCAS and ECIS) are used. To achieve that we have considered a simple potential for the description of the nucleon-^{12}C dynamics which includes low-lying excitations of the target in terms of a collective, rotational-type model where the quadrupole deformation β_2 has been set to a (realistic) value of -0.52. Within the unavoidable small differences that remain in the construction of the programs, for this particular case we have shown that the results of the two approaches are essentially equivalent.

However, with the MCAS approach we could include also the effects of second-order contributions in the deformation parameter. They lead to substantial changes to the cross section. Even more importantly, with the MCAS approach we could eliminate the spurious states that appear if one ignores the effects of the Pauli principle with the Schrödinger equation. In the MCAS method one can take account of the effects due to the identity between the projectile nucleon and the nucleons in the target by applying a suitable generalization of the orthogonalizing pseudo-potential method. The effects due to Pauli principle are very significant; greatly influencing the overall structure of the cross-section and changing completely the resonant and bound spectra of the compound system associated with a fixed interaction.

A distinctive feature of the MCAS approach is that, by study of the spectra as $\beta_2 \to 0$, it allows the unphysical nature of the spurious states to be illustrated. Doing that in a previous study [11] emphasized the need for their elimination from the coupled-channel dynamics.

Another interesting feature of the MCAS approach is that one can systematically track all resonances and bound-state structures contained in the compound system. This feature is particularly welcome for the specific problem we have considered and is a consequence of the use of Sturmian states in the expansion scheme. Even the most narrow resonant scattering state can be numerically determined, its spin-parity and width can be easily evaluated without the need to organize an extremely fine (and extremely time consuming) energy spanning of the S-matrix to seek rapid increases in phase shifts. Closely related to this property is the capacity to assess the order number of a given resonance which indicates how many other resonances and bound states with the same spin and parity lie below the one considered. This parameter is important within the process of data evaluation, since fitting procedures in coupled-channel calculations that ignore the need for dealing with an entire ensemble of physical states (without spurious entries) have very little physical relevance.

In summary, the MCAS approach, albeit still in its infancy, is a promising means to study low energy nuclear reaction cross sections since it allows treatment of the Pauli principle in a simple manner, it facilitates solution of sub-threshold spectra as well as defining resonance behavior due to coupled-channel effects, and encompasses a procedure which finds all resonances produced in the selected energy interval. On the other hand, the coordinate space coupled-channels programs currently in use need upgrading at least to incorporate effects of the Pauli principle before their interactions and associated relative motion wave functions may be used with confidence of physical significance. Whether some scheme, such as supersymmetric quantum mechanics, can be found to effect that upgrade is a major problem for developers and users of those codes.

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